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Electron optical phase-shifts by Fourier methods: Analytical versus numerical calculations

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Abstract

The theoretical framework for the computation of electromagnetic fields and electron optical phase-shifts in Fourier space has been recently applied to objects with long-range fringing fields, such as reverse-biased p–n junctions and magnetic stripe domains near a specimen edge. In addition to new analytical results, in this work, we present a critical comparison between numerical and analytical computations. The influence of explicit and implicit boundary conditions on the phase shifts and phase-contrast images is also investigated in detail.

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1. Introduction

In a previous work [1], hereafter referred to as I, we have applied a Fourier-space formalism to the computation of the electron optical phase-shift associated to long-range electric and magnetic fields. In particular, we have analysed in detail a one-dimensional p–n junction described by the Spivak or step model, a semi-infinite array of reverse-biased step p–n junctions and a semi-infinite array of magnetic stripe domains. It should be mentioned that this approach was formerly introduced for the calculation of the electron optical phase-shifts and phase-contrast images of superconducting fluxons [2–4]. Then, it was extended to cover magnetic nano-structures [5,6], leading to a new description of shape anisotropy effects in nano-particles [7,8] and to a connection

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between micro-magnetic simulations and phase computations [9].

Following a structure similar to I, in this work, we present the results of our most recent studies, aimed at further exploiting the analytical capabilities of the method and to investigate the relationship between analytical and numerical calculations of the phase-shifts and phase-contrast images. In particular, it is shown how, in the case of one-dimensional reverse-biased p–n junctions, the Fourier approach allows the recovering of the analytical expression for the phase when even more realistic models for the junction field topography are considered, like, e.g. the parabolic model. By including also the presence of contacts at a finite distance from the junction it is possible to investigate what happens when this distance increases and hence have a better understanding of the effects introduced by the finiteness of the specimen.

For the two-dimensional case the main result is represented by the analytical expression obtained for the phase shift of the Fourier components, thus eliminating the Gibbs phenomenon arising in the former numerical inversion. Also a different but closely related boundary value problem has been considered, which shows how phase maps are influenced by the chosen model.

Although the former issues might appear rather abstract and academic, problems of this kind are often occurring in the interpretation of TEM phase-contrast images of p–n junctions. As electron microscopy is playing an increasingly relevant role in the characterization of the junctions and the extraction of dopant profile information is a key point in the semiconductor road-map [10], a sound theoretical background is necessary in order to be confident in the results inferred from the interpretation of the images. In this respect, the presented solution of the half-plane problem can be considered a first approximation to the truly three-dimensional analysis of the observed device (which can probably carried out only by a numerical approach) and as such useful both as a test reference and as an analytical approximation of the numerical solution.

Finally, the same procedure is applied to magnetic specimens, where additional field topographies have been considered: in this case the influence of the external and demagnetizing fields on the phase maps and phase-contrast (out-of-focus) images has been taken into account. The results confirm that phase maps are not very representative of the magnetization trend within the specimen but nonetheless give a broad two-dimensional view of it, whereas out-of-focus images, more sensitive to the gradient of the phase, correctly indicate the position of the domain walls, but do not give reliable information about the magnetization inside the domains. It is also shown how the finite size of the micro-magnetic numerical calculations does not properly take into account the external field and can introduce non-negligible errors (up to 20%) in the calculation of the phase.

2. General considerations

Let us recall, for the sake of completeness, the main conventions and general results obtained in I. The specimen is considered in the form of a thin slab of constant thickness t, supporting charges and currents, i.e. the sources of electric and magnetic fields respectively, which may extend in the whole space. The microscope coordinate system has the z-axis parallel to the electron beam and aligned in the same direction, whereas x and y are the coordinates in the object plane, perpendicular to the optical axis [11,12]. The origin of our coordinate system is the intersection of the optical axis with the mid-plane of the specimen. The object wave-function $\psi(x,y)$ is given by

$$\psi(x,y) = a(x,y)\exp[\mathrm{i}\varphi(x,y)], \tag{1}$$

where $a(x,y)$ is the amplitude term (hereafter assumed equal to one, i.e. no absorption) and the phase $\varphi(x,y)$ is given by

$$\varphi(x,y) = \frac{\pi}{\lambda E}\int_{\ell} V(x,y,z)\,\mathrm{d}z - \frac{2\pi e}{h}\int_{\ell} A_z(x,y,z)\,\mathrm{d}z. \tag{2}$$

The integral is taken along a trajectory ℓ parallel to the optical axis z inside and outside the specimen to include stray fields, $V(x,y,z)$ and $A_z(x,y,z)$ are the electrostatic potential and the z-component of